BENCH MARK

Setting the Analysis Agenda

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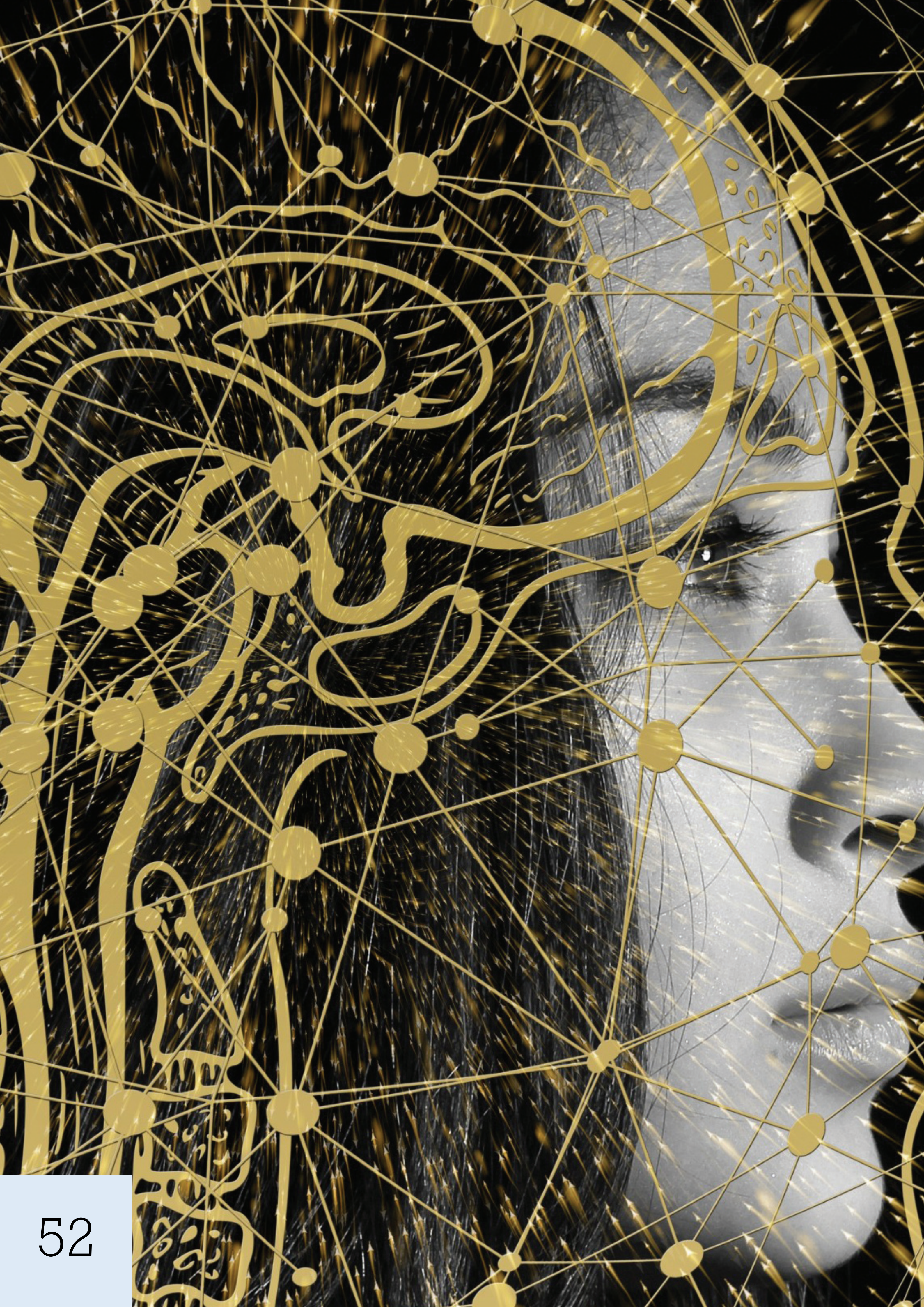


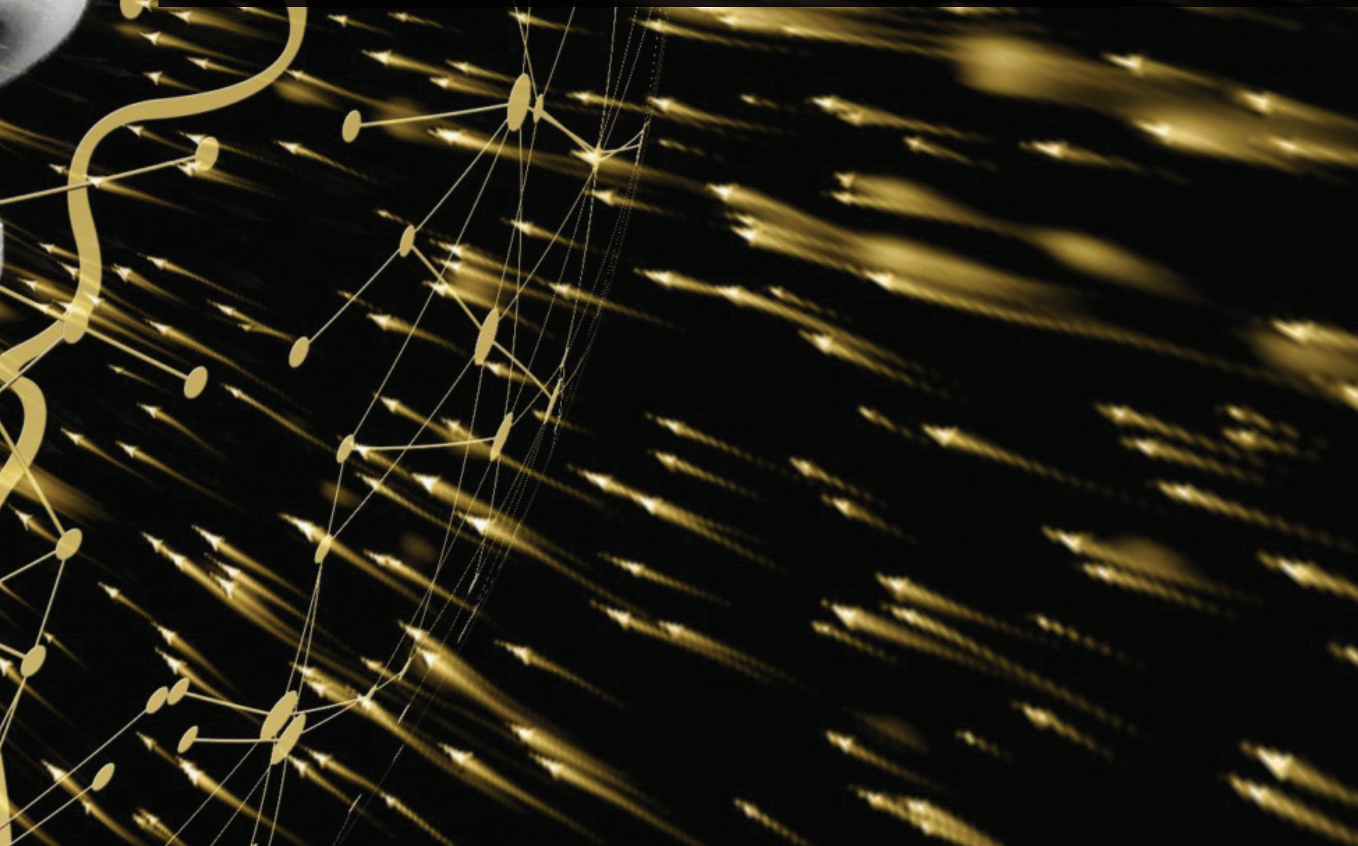
AI, Data Driven Models & Machine Learning:

How Will Advanced Technologies Shape Future Simulation Processes?

A Summary of the Recent NAFEMS Workshop

Mahmood Tabaddor | Underwriters Laboratories LLC

Recognizing the growing influence of Machine Learning (ML), a technology contributing to Artificial Intelligence (AI), NAFEMS organized a workshop entitled “AI, Data Driven Models & Machine Learning: How Will Advanced Technologies Shape Future Simulation Processes?” in late April of 2021. As an organization committed to advancing the use of engineering simulation technologies, the availability of ML has made it a viable technology that can be part of the engineering simulation toolkit. To help our membership filter through the hype, the workshop included a diverse group of speakers representing current and practical uses of machine learning in support of product development and design.



Several themes governed the overall content and focus of the workshop. One theme was how traditional engineering simulations and ML can, together, help deliver productivity gains. Another theme was model trustworthiness, and how ML algorithms provide a greater challenge than traditional engineering simulation in demonstrating that their predictions can be trusted. And the last theme was on Physics Informed Machine Learning.

In planning the workshop, the NAFEMS organizing team wanted to help create opportunities to network during an online meeting. Trying to match the spontaneous and unplanned conversations typical of a physical conference is challenging. For this workshop, in addition to the standard speaker presentations, there were two opportunities for engagement. One was the concept of breakout rooms and the other was an interactive panel discussion as the last activity for the two-session workshop.

Breakout rooms allow for groups of up to ten participants to engage in a conversation on a topic of their choice. Some of the breakout rooms had a topic pre-selected and facilitator while others remained open for spontaneous gathering. The 1-hour breakout room topics for Day 1 of the workshop included: "Differential Equations and Data Driven Models: Which one came first and which one is more reliable for engineering practices?" facilitated by Kambiz Kayvantash (CADLM); "Learn to Predict, or Learn to Simulate? Big Data, or Small Data? -- Reality in the Simulation World" facilitated by Zhenyuan Gao (Dassault Systèmes SIMULIA); "How to Trust ML/AI Algorithms?" facilitated by Mahmood Tabaddor (UL LLC) and "The Best AI is Invisible. Would you agree?" facilitated by Fatma Kocer (Altair Engineering).

For Day 2 of the workshop, breakout room topics included "How will real-time simulations impact the products around us?" facilitated by Anthony Massobrio (Neural Concept Ltd.); "What steps should I take to determine how my team might best utilize AI data driven models and the digital twin concept?" facilitated by Rod Dreisbach (IEAC); "How is AI impacting the way we should train tomorrow's engineering simulation workforce?" facilitated by Olivia Pinon Fischer (Aerospace Systems Design Laboratory); "Is physics based knowledge the future of ML/AI? What is 'Small Data' and are we at the cusp of a revolution in ML/AI?" facilitated by Juan Betts (Front End Analytics); and finally, "Autoencoders: Are they the future of ROM and generative design?" facilitated by Marc Emmanuelli (Monolith AI).

For the theme of Physics-Informed Machine learning, Tobias Pffaf (DeepMind) talked about research in the area of PIML and more specifically the use of Graph Network to help "learn simulation" in his talk entitled "Learning Simulation Using Graph Networks". One of the key benefits is that the speed of simulation for PIML will generally be much faster than traditional engineering simulation. However, the downside is the concern with extrapolation as ML based models, especially neural networks, will be less accurate than traditional engineering simulation methods.

This work focused on the learning of reusable knowledge, similar to the laws of physics, to allow for the use of the model outside of the training data set. Tobias showed some of the research demonstrating the possibility for learning simulations using examples from structural mechanics, particle dynamics, aerodynamics, and even cloth dynamics. Though he emphasized the early nature of this work, he has shown that it is possible to overcome the challenge of generalization of a model beyond its trained data by narrowing the domain of interest. As the scale of the problem becomes larger, the benefits of the speed of such techniques may further advances in this area.

In contrast to PIML, the next theme was not about replacing engineering simulation with ML based technologies, rather it was about the data used for training coming from traditional engineering simulation generated data. Peter Chow (Fujitsu) opened the workshop with his talk on "AI for Simulation: Current Possibilities and Future Challenges" where he gave very practical examples such as 3D shape search and classification of PCBs. One topic was how ML can be trained on data generated by traditional engineering simulation to help create a reduced order model (ROM). ROMs are generally computationally less intensive to run but come at the cost of less detailed insight into the entire domain.

Use cases cited by several speakers, including Peter Chow as well as Robin Tuluie (Physics X) in his talk "Data Science Driving the Future of Engineering Simulation", covered examples of ROMs developed in the different physics domains from heat transfer and aerodynamics to electromagnetics and structural modeling. In addition to the main stage speakers, case study speakers also tackled this topic with talks such as "The New 'AI' Wave: Does it Apply to Engineering?" by Pierre Baqué (Neural Concept Ltd.), "AI-Powered Product Design" by Fatma Kocer "AI/ML/ROM-based Modeling, Prediction and Optimization for CAE Applications" by Kambiz Kayvantash (CADLM), and a talk by Yangzhan Yang (Dassault Systèmes SIMULIA) on "Combining Machine Learning and Physics-based Simulation for Product Development".

Other pertinent areas of AI & ML were also covered by Mohan Varma (VCollab) on the use of ML for modeling efficiencies in a case study entitled "Machine Learning for Automation of CAE Post-processing and Report Generation", and by Danilo Di Stefano and Marco Turchetto (ESTECO) on how ML methodologies can be applied to engineering simulation data in a case study entitled "Best Practices for Data Driven Simulation Modelling".

Joshua Stuckner (NASA Glenn) gave a talk on "Efficient Multiscale Composite Modeling via an Embedded Long Short Term Memory Surrogate Microscale Model" where he went through a detailed explanation on the use of LSTM neural networks to help create a fast and accurate representation of a micromechanics model of a composite structure. Even he ended with the caution, "careful how the model is used".

This brings us to the last theme, the topic of model trustworthiness. In the talk entitled "The Challenge with Trustworthiness of Data Driven and Machine Learning Approaches" by Mahmood Tabaddor (UL LLC) a parallel was drawn between the need for an equivalent "model verification and validation" initiative for ML based models similar to that for traditional engineering simulation. In addition to this talk, the 2-session workshop ended with a panel discussion on the "State of Explainable AI/ML". The panel consisted of Olivia Pinon Fischer, Peter Chow, Robin Tuluie, and Ankit Patel (Rice University), and was facilitated by Mahmood Tabaddor. The panel addressed two main questions: "Is the opaque nature of some ML models a showstopper (and what are the risks of using a blackbox model)?" and "What are some practical tools and techniques for Explainable AI (XAI)?".

Ultimately, one sign of a workshop's success is the number of attendees and the feedback. There were over 200 attendees representing a global presence from South Korea to India to Kuwait. The interest shown by the attendees was captured in the high rating given to the quality and relevance of the presentations. Another important metric is sponsorship, which included companies such as Hexagon | MSC Software, VCollab, Dassault Systèmes SIMULIA, ESTECO, Altair Engineering, Front End Analytics, and some new non-traditional sponsors such as Monolith AI and Neural Concept Ltd. Overall, ML is following growing pains similar to traditional engineering simulation and NAFEMS is well positioned to help its members understand and add ML technologies as a practical tool to aid their company's design processes and deliver more innovative products.

Acknowledgemnts

We'd like to thank all our presenters and participants for making this another stand-out NAFEMS event. We are also grateful to the event sponsors: Hexagon/MSC, Vcollab, Dassault Systèmes Simulia, ESTECO, Neural Concept, Altair, Front End Analytics and Monolith.

Mahmood Tabaddor has degrees in Mechanical Engineering from University of Michigan, Ann Arbor and Engineering Mechanics from Virginia Tech, and has been involved in modeling and simulation for over 25 years. He has published papers and given presentations on how modeling has given insights into a wide range of problems.

He formed the first modeling and simulation team within Underwriters Laboratories (UL), a leader in testing, inspection and certification, and is currently a member of the NAFEMS Americas Steering Committee.